Rational approximation to the Thomas–Fermi equation

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May 28, 2008

Abstract

We discuss a recently proposed analytic solution to the Thomas–Fermi (TF) equation and show that earlier approaches provide more accurate results. In particular, we show that a simple and straightforward rational approximation to the TF equation yields the slope at origin with unprecedented accuracy, as well as remarkable values of the TF function and its first derivative for other coordinate values.

1 Introduction

The Thomas–Fermi (TF) equation has proved useful for the treatment of many physical phenomena that include atoms [1–5], molecules [3,6], atoms in strong magnetic fields [1,4,5], crystals [7] and dense plasmas [8] among others. For that reason there has been great interest in the accurate solution of that equation, and, in particular, in the accurate calculation of the slope at origin [9–11]. Besides, the mathematical aspects of the TF equation have been studied in detail [14, 15]. Some time ago Liao [16] proposed the application of a technique called homotopy analysis method (HAM) to the solution of the TF equation and stated that "it is the first time such an elegant and

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explicit analytic solution of the Thomas–Fermi equation is given". This claim is surprising because at first sight earlier analytical approaches are apparently simpler and seem to have produced much more accurate results [10–13]. Recently, Khan and Xu [17] improved Liao's HAM by the addition of adjustable parameters that improve the convergence of the perturbation series.

The purpose of this paper is to compare the improved HAM with a straightforward analytical procedure based on Padé approximants [13] supplemented with a method developed some time ago [18–26]. In Section 2 we outline the main ideas of the HAM, in Section 3 apply the Hankel–Padé method (HPM) to the TF equation, and in Section 4 we compare the HAM with the HPM and with other approaches.

2 The homotopy analysis method

In order to facilitate later discussion we outline the main ideas behind the application of the HAM to the TF equation. The TF equation

$$u''(x) = \sqrt{\frac{u(x)^3}{x}},\ u(0) = 1,\ u(\infty) = 0 \tag{1}$$

is an example of two–point nonlinear boundary–value problem. When solving this ordinary differential equation one faces problem of the accurate calculation of the slope at origin $u'(0)$ that is consistent with the physical boundary conditions indicated in equation (1).

In what follows we choose the notation of Khan and Xu [17] whose approach is more general than the one proposed earlier by Liao [16]. They define the new solution $g(\xi) = \gamma u(x)$, where $\xi = 1 + \lambda x$ and rewrite the TF equation as

$$(\xi - 1)\lambda^3 \gamma g''(\xi)^3 - g(\xi)^3 = 0 \tag{2}$$

where γ is the inverse of the slope at origin ($u'(0) = 1/\gamma$) and λ is an adjustable parameter. Khan and Xu [17] state that the solution to Eq. (2) can be written in the form

$$g(\xi) = \sum_{j=1}^{\infty} A_j \xi^{-j} \tag{3}$$

that reduces to Liao's expansion [17] when $\lambda = 1$.

In principle there is no reason to assume that the series (3) converges and no proof is given in that sense [16, 17]. Besides, the partial sums of the series (3) will not give the correct asymptotic behaviour at infinity [14, 15, 27] as other expansions do [10, 11].

Liao [16] and Kahn and Xu [17] do not use the ansatz (3) directly to solve the problem but resort to perturbation theory. For example, Kahn and Xu [17] base their approach on the modified equation

$$(1-q)\mathcal{L}\left[\Phi(\xi;q)-g_0(\xi)\right]=q\hbar\mathcal{N}\left[\Phi(\xi;q),\Gamma(q)\right] \tag{4}$$

where $\mathcal{L}$ and $\mathcal{N}$ are linear and nonlinear operators, respectively, $0 \leq q \leq 1$ is a perturbation parameter and $\hbar$ is another adjustable parameter. Besides, $g_0(\xi)$ is a conveniently chosen initial function and $\Phi(\xi;q)$ becomes the solution to equation (2) when $q=1$ [17]. Both $\Phi(\xi;q)$ and $\Gamma(q)$ are expanded in a Taylor series about $q=0$ as in standard perturbation theory, and $\Gamma(0)=\gamma_0$ is another adjustable parameter [17].

The authors state that HAM is a very flexible approach that enables one to choose the linear operator and the initial solution freely [16, 17] and also to introduce several adjustable parameters [17]. However, one is surprised that with so many adjustable parameters the results are far from impressive, even at remarkable great perturbation orders [16,17]. For example the [30/30] Padé approximant of the HAM series yields $u'(0)$ with three exact digits [17], while the [1/1] Padé approximant of the δ expansion [28] provides slightly better results [29, 30]. A more convenient expansion of the solution of the TF equation leads to many more accurate digits [10, 11] with less terms.

3 The Hankel–Padé method

In what follows we outline a simple, straightforward analytical method for the accurate calculation of $u'(0)$. In order to facilitate the application of the HPM we define the variables $t=x^{1/2}$ and $f(t)=u(t^2)^{1/2}$, so that the TF equation becomes

$$T(f,t)=t\left[f(t)f''(t)+f'(t)^2\right]-f(t)f'(t)-2t^2f(t)^3=0 \tag{5}$$

We expand the solution $f(t)$ to this differential equation in a Taylor series about $t=0$:

$$f(t)=\sum_{j=0}^{\infty}f_jt^j \tag{6}$$

where the coefficients f_j depend on $f_2 = f''(0)/2 = u'(0)/2$. On substitution of the series (6) into equation (5) we easily calculate as many coefficients f_j as desired; for example, the first of them are

$$f_0 = 1,\ f_1 = 0,\ f_3 = \frac{2}{3},\ f_4 = -\frac{f_2^2}{2},\ f_5 = -\frac{4f_2}{15}, \ldots \tag{7}$$

The HPM is based on the transformation of the power series (6) into a rational function or Padé approximant

$$[M/N](t) = \frac{\sum_{j=0}^{M} a_j t^j}{\sum_{j=0}^{N} b_j t^j} \tag{8}$$

One would expect that $M < N$ in order to have the correct limit at infinity; however, in order to obtain an accurate value of f_2 it is more convenient to choose $M = N + d$, $d = 0, 1, \ldots$ as in previous applications of the approach to the Schrödinger equation (in this case it was called Riccati–Padé method (RPM)) [18–26].

The rational function (8) has $2N+d+1$ coefficients that we may choose so that $T([M/N], t) = \mathcal{O}(t^{2N+d+1})$ and the coefficient f_2 remains undetermined. If we require that $T([M/N], t) = \mathcal{O}(t^{2N+d+2})$ we have another equation from which we obtain f_2. However, it is convenient to proceed in a different (and entirely equivalent) way and require that

$$[M/N](t) - \sum_{j=0}^{2N+d+1} f_j t^j = \mathcal{O}(t^{2N+d+2}) \tag{9}$$

In order to satisfy this condition it is necessary that the Hankel determinant vanishes

$$H_D^d = \left| f_{i+j+d+1} \right|_{i,j=0,1,\ldots N} = 0, \tag{10}$$

where $D = N + 1$ is the dimension of the Hankel matrix. Each Hankel determinant is a polynomial function of f_2 and we expect that there is a sequence of roots $f_2^{[D,d]}$, $D = 2, 3, \ldots$ that converges towards the actual value of $u'(0)/2$ for a given value of d. We compare sequences with different values of d for inner consistency (all of them should give the same limit). Notice that a somewhat similar idea was also proposed by Tu [12], although he did not develop it consistently.

Present approach is simple and straightforward: we just obtain the Taylor coefficients f_j from the differential equation (5) in terms of f_2, derive the

Hankel determinant, and calculate its roots. Since f_4 is the first nonzero coefficient that depends on f_2 we choose Hankel sequences with $d \geq 3$.

The Hankel determinant H_D^d exhibits many roots and their number increases with D. If we compare the roots of H_D^d with those of H_{D-1}^d we easily identify the sequence $f_2^{[D,d]}$ that converges towards the actual value of f_2. Fig. 1 shows $\log \left| 2f_2^{[D,d]} - 2f_2^{[D-1,d]} \right|$ for $D = 3, 4, \ldots$ that provides a reasonable indication of the convergence of the sequence of roots. We clearly appreciate the great convergence rate of the sequences with $d = 3$ and $d = 4$. For example, for $d = 3$ and $D \leq 30$ it is approximately given by $\left| 2f_2^{[D,3]} - 2f_2^{[D-1,3]} \right| = 14.2 \times 10^{-0.705D}$. From the sequences for $D \leq 30$ we estimate $u'(0) = -1.588071022611375\,31$ which we believe is accurate to the last digit. We are not aware of a result of such accuracy in the literature with which we can compare our estimate. It is certainly far more accurate than the result obtained by Kobayashi et al [9] by numerical integration that is commonly chosen as a benchmark [16, 17].

Present rational approximation to the TF function is completely different from previous application of the Padé approximants, where the slope at origin was determined by the asymptotic behaviour of at infinity [13]. Our approach applies to $u(x)^{1/2}$ and the slope at origin is determined by a local condition at that point (9) which results in the Hankel determinant (10). In this sense our approach is similar to (although more systematic and consistent than) Tu's one [12] as mentioned above.

Once we have the slope at origin we easily obtain an analytical expression for $u(x)$ in terms of the rational approximation (8) to $f(t)$. In order to have the correct behaviour at infinity we choose $N = M + 3$ [13]. Table 1 shows values of $u(x)$ and its first derivative for $1 < x < 1000$ (the approximation is obviously much better for $0 < x < 1$) given by the approximant [5/8]. Our results are in remarkably agreement with the numerical calculation of Kobayashi et al [9] and are by far much more accurate than those provided by the HAM [16, 17]. Notice that we are comparing a [5/8] Padé approximant on the straightforward series expansion (6) with [50/50] and [30/30] approximants on an elaborated perturbation series [16, 17].

4 Conclusions

Any accurate analytical expression of the solution $u(x)$ to the TF equation requires an accurate value of the unknown slope at origin $u'(0)$, and the HPM

provides it in a simple and straightforward way. In this sense the HPM appears to be preferable to other accurate approaches [9–11] and is far superior to the HAM [16, 17]. Notice for example that our estimate $2f_2^{[5,3]} = -1.588$, based on a rational approximation [7/4], is better than the result provided by a [30/30] Padé approximant on the improved HAM perturbation series [17]. Besides, by comparing Table 2 of Khan and Xu [17] with our Fig. 1 one realizes the different convergence rate of both approaches. One should also take into account that the HPM does not have any adjustable parameter for tuning up its convergence properties, while, on the other hand, the "flexible" HAM with some such parameters plus a Padé summation results in a much smaller convergence rate [16, 17].

We also constructed a Padé approximant [5/8] from the series (6) and obtained the TF function and its derivative with an accuracy that outperforms the [50/50] and [30/30] Padé approximants on the HAM perturbation series [16, 17]. It is clear that the HPM is by far simpler, more straightforward, and much more accurate than the HAM.

In addition to the physical utility of the HPM we think that its mathematical features are most interesting. Although we cannot provide a rigorous proof of the existence of a convergent sequence of roots for each nonlinear problem, or that the sequences will converge towards the correct physical value of the unknown, a great number of successful applications to the Schrödinger equation [18–26] suggest that the HPM is worth further investigation. Notice that we obtain a global property of the TF equation $u'(0)$ from a local approach: the series expansion about the origin (6). The fact that our original rational approximation (8) does not have the correct behaviour at infinity is not at all a problem because we may resort to a more conventient expansion [13] once we have an accurate value of the unknown slope at origin.

Finally, we mention that the HPM has recently proved successful for the treatment of other two–point nonlinear equations [31] of interest in some fields of physics [32–34].

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Table 1: Values of the Thomas-Fermi function and its derivative

x	$u(x)$	$-u'(x)$
1	0.424008	0.273989
5	0.078808	0.023560
10	0.024315	0.0046028
20	0.005786	0.00064727
30	0.002257	0.00018069
40	0.001114	0.00006969
50	0.000633	0.00003251
60	0.000394	0.0000172
70	0.0002626	0.000009964
80	0.0001838	0.000006172
90	0.0001338	0.000004029
100	0.0001005	0.000002743
1000	0.000000137	0.00000000040

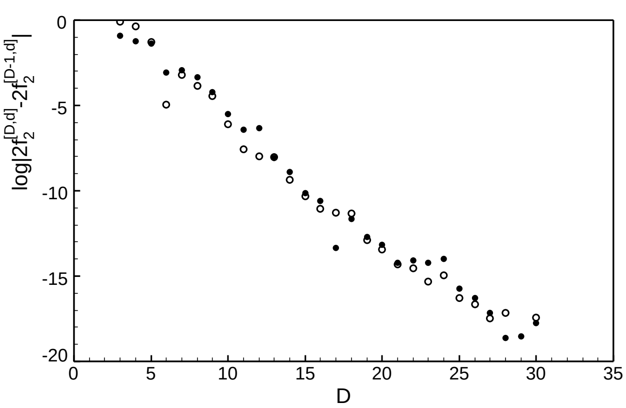

Figure 1: $\log\left|2f_2^{[D,d]} - 2f_2^{[D-1,d]}\right|$ for $d = 3$ (circles) and $d = 4$ (filled circles)